

COLLISIONAL-RADIATIVE MODELING OF FREE-BURNING ARC PLASMA IN ARGON

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Abstract

Recent ambitions have been aimed at improving a free-burning arc modeling by means of a self-consistent description of the arc plasma and the electrodes avoiding assumptions of equilibrium. As next step, the present work is dealing with the impact of the reaction chemistry used in non-equilibrium modelling of free-burning arc in argon. A simple chemistry model based on the approximation of prompt ionization, a model with an effective excited level, and a model implying higher excited levels of argon atoms are considered. The results obtained show that all three models are capable of predicting the arc characteristics. They deliver values of electric current density, electric conductivity, arc voltage, electron and heavy particle temperature which are close to each another. The simple model can serve as a fast track evaluation of the arc characteristics, and for sensitive studies of the impact of model parameters. The extended model allows obtaining the populations of individual and effective levels giving rise to important radiative transitions and enables comparisons with spectroscopic measurements.

I. INTRODUCTION

The non-equilibrium modelling of arc plasmas is a problem of increasing interest. A series of investigations during the last two decades were aimed at describing the deviations from local thermodynamic equilibrium (LTE) in the near-electrode regions in the frame of two-temperature hydrodynamic models accompanied by sheath-accounting approaches (see e.g. [1-4]). The role of the near-cathode sheath plays has been found to be important [5 and references therein]. In a recent paper [6], a self-consistent non-equilibrium model of a free-burning arc in argon was presented. An important highlight of the model was the unified description of the whole plasma domain avoiding the division into sub-domains in which different models were used and the subsequent coupling of the solutions. The results showed that the non-equilibrium model provided a realistic description of the near-electrode regions, the current transfer and the plasma

properties. Furthermore, a deviation from the chemical non-equilibrium even in regions of equal temperatures of electrons and heavy particles was demonstrated.

The plasma chemistry is important but yet just one element of the complex arc description. Therefore, the present work is aimed at the analysis of the plasma chemistry in a way that the model enables a deeper look into the populations of excited states keeping computation costs still reasonable. From one site the populations of the excited states are of interest in the evaluation of the emission spectra and the spectroscopic validation of the model. From the other site, excited atoms play an important role in the kinetics of production and loss of charged particles. The main objective is to find a chemistry model which is capable of predicting proper plasma characteristics and distribution of atoms over the excited states.

Under a wide range of conditions, the total particle density of excited states is much less compared with the ground state and the electron number density. The ground and the continuum states can be considered as pools of particles and the particle flow between them goes through the excited states. The distribution of atoms over their excited states can be obtained by means of a collisional-radiative (CR) model. A review on CR models in plasmas is given e.g. in [7]. Numerous CR models of argon plasma have been reported over the years applicable to a variety of conditions (see for example [8-17]). In these models, the electron energy distribution function was assumed to be Maxwellian or it was obtained by solving the Boltzmann equation for the electrons. The models differ in the number of excited states or groups of states included to represent the discrete atomic structure.

However, a typical assumption for the excited states is that the contribution of populating and depopulating CR processes is large compared to the corresponding convective and diffusive terms. Therefore, the densities of the excited states are obtained in the frame of the quasi-stationary formulation [18] as the equation system is solved for given electron density and temperature (provided that a Maxwellian distribution is considered). The densities of the excited states are then conveniently expressed as functions of the ground state atomic density and the electron density through the so-called collisional-

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radiative effective ionization and recombination coefficients.

Another approach to obtain ionization and recombination coefficients is based on the electron diffusion during recombination (ionization) in the energy space which is assumed continuous [19]. It is well justified for the highly excited states where the energy levels are closely spaced. A modified diffusion approximation combines the real level structure and the diffusion approach and can also account for radiation processes. In order to simplify the description in place of real levels a small number of levels is considered so that the lower-lying levels are included and the higher levels are ignored or combined into one or more levels characterized by artificially high degeneracies to ensure a particle flow into the continuum [7, 20-22]. This scheme is suitable for argon plasma since the energy gap between the ground state and the first excited state is large.

In the “bottleneck” model [22,23], a part of the excited states is assumed in equilibrium with the ground state and the higher lying levels are in equilibrium with the continuum. The recombination rate is determined by the rate of transition of the recombining electron between the two groups. The position of the bottleneck changes depending on the plasma parameters. At electron temperatures below 3000 K, the “bottleneck” lies in the highly excited states [24]. The recombining electron reaches the ground state quickly and the level structure below the “bottleneck” is insignificant. With increasing electron temperature the bottleneck moves to the low lying levels. The main contribution to the recombination is due to the transition between the ground state and the first excited state so that the approximation of the prompt ionization is valid.

For the system of neutral atomic argon which is of interest in the present work, the CR model shall treat excitation and de-excitation, ionization, recombination and radiative processes which occur in a free-burning arc. The excited states are grouped in effective levels in order to reduce the computational costs though yielding a realistic plasma parameters and populations of the excited states.

II. THE ARC MODEL

The basic concept of the arc model used in the present work is similar to that of [6] and shall be briefly presented in the following. A tungsten inert gas (TIG) arc at normal pressure is burning between a tungsten cathode with a conical tip and a water cooled flat copper anode. The computational domain includes the arc region, the electrodes, and a part of the nozzle (Fig. 1). It is 21 mm radially by 21 mm axially employing rotational symmetry around the x -axis within a pie-slice of 10° . The cathode has a radius of 2 mm and the flattened part of its conical tip has a radius of 0.2 mm. The distance between the cathode and the anode is 8 mm. The arc current is 200 A.

A gas flow is supplied through the nozzle (the patch on the passage AB) with a flow rate of 12 slpm.

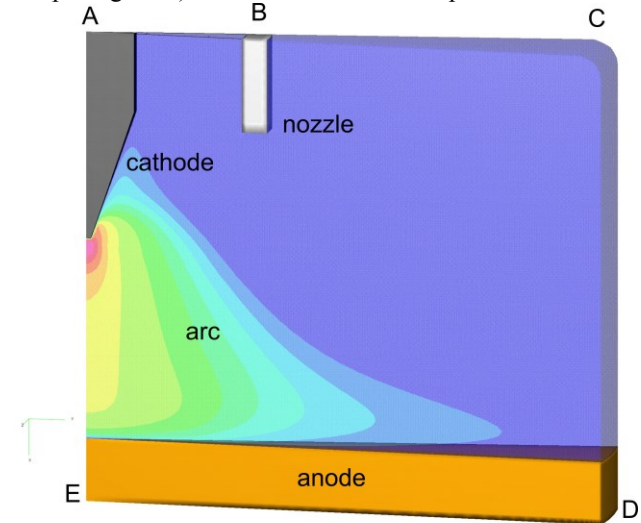


Figure 1. Schematic view of the computational domain.

The system including the arc and the electrodes is simulated by means of a self-consistent non-equilibrium model based on the magnetohydrodynamic approach. The plasma behaves like a fluid consisting of electrons and heavy particles of argon (ground state atoms, excited atoms, and atomic ions). Reaction schemes with an increasing level of complexity are used in the model and are considered below. The heavy particles are assumed to be in thermal equilibrium at a temperature T , and the electrons are characterized by a Maxwellian energy distribution function with a temperature T_e ($T_e \neq T$). Melting effects and metal vapor from the weld pool are not included.

In the hydrodynamic model, the Navier-Stokes equations provide a solution for the total mass density and the mass-averaged velocity. Separate energy conservation equations are solved for heavy particles and electrons. The continuity equation of electric current supplemented with Ohm's law and Maxwell's equations are considered to obtain the electric potential, and the self-induced magnetic field. The species transport is described by diffusion equations for the excited atoms and ions. The heat transport in the electrodes accounts for thermal conduction and Joule heating. The model is closed by means of boundary conditions similar to those in [6]. The unified description of the plasma and the electrodes is realized implementing a sheath model, in which the space charge sheath is treated as a zero-dimensional interface and the plasma characteristics of the pre-sheath are obtained from the near-surface control volumes of the arc plasma model. The energy balance of the electrodes is completed taking into account the energy fluxes on their boundaries with the plasma due to ion and electron heating, electron emission and black body radiation. The model is developed using the customized commercial code CFD-ACE+[25].

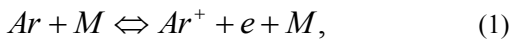
III. PLASMA CHEMISTRY

The present study aims at analyzing the collisional and radiative processes in argon with a view toward application to non-equilibrium modeling of a free-burning arc. Considering simultaneously both chemical and thermal non-equilibrium, a satisfactory model must combine physically realistic rate expressions for electron production and recombination with an appropriate electron energy balance. The basic mechanisms of production and loss of electrons in argon according to [26] are electron-atom collisions, atom-atom collisions, photo-ionization, and recombination.

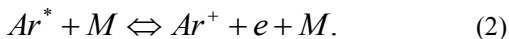
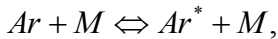
A transport equation for the ions and the excited states is solved in the arc model (see Ch. II). In the general case of an arbitrary number of excited levels, the production of ions occurs by collisions with electrons and atoms from all levels whereas the losses comprise three-body recombination to the 4s-levels according to the "bottleneck" concept [22] and radiative recombination of electrons and ions to the excited states [9].

The processes considered in the plasma chemistry contribute to the energy equations for heavy particles and electrons. The heat release due to non-electronic collisions is expressed through the species enthalpy and the stoichiometric coefficients of the products and reactants. The electron energy loss in inelastic collisions is expressed through the products of the electron number density, the corresponding heavy species density, and the energy loss of the process. The loss of electron energy due to elastic collisions with heavy species equals the gas heating due to elastic collisions. It is expressed by means of the frequency for momentum transfer, the temperature difference between the electron temperature and the temperature of heavy species, and the masses of the corresponding species. A description of the individual terms is given in great detail in [6].

In the frame of the simplest reaction chemistry which will be referred to as "simple model", a two-level representation of the atomic argon energy structure is considered. The model describes species of a ground state level and an ion state. The collisional ionization kinetics is considered to take place following the overall reaction



where M denotes an electron (e) or argon atom (Ar) [27]. The reactions given with Eq. (4) implicitly consist of two reaction steps implying atoms in the first excited state or the group of the four lowest 4s-excited states (Ar^*):



Upper levels are not considered since the "bottleneck" is assumed to move to the lowest excited level so that the approximation of the prompt ionization is applied considering the first reaction in Eq. (1) as rate-controlling. The rate coefficients for ionization and recombination in collisions with electrons ($M=e$) used in

the models presented here are written as follows [20,23,24,27]:

$$K_{i,e} = 2.82 \times 10^8 T_e [eV]^{1.5} \left(\frac{135300}{T_e [K]} + 2 \right) \times \exp \left(- \frac{135300}{T_e [K]} \right) [m^3 (mol \cdot s)] \quad (3)$$

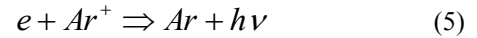
$$K_{3+,e} = \begin{cases} 3.17 \times 10^9 T_e [eV]^{-4.5} [m^6 / (mol^2 \cdot s)], & T_e \leq 0.26 eV \\ 4.68 \times 10^3 \left(\frac{135300}{T_e [K]} + 2 \right) \exp \left(\frac{47800}{T_e [K]} \right) [m^6 / (mol^2 \cdot s)], & T_e > 0.26 eV. \end{cases}$$

The rate coefficients for ionization and recombination in collisions with argon atoms ($M=Ar$) are given as [27]

$$K_{i,a} = 1.26 \times 10^4 T [eV]^{1.5} \left(\frac{135300}{T [K]} + 2 \right) \times \exp \left(- \frac{135300}{T [K]} \right) [m^3 / (mol \cdot s)] \quad (4)$$

$$K_{3+,a} = 0.21 \left(\frac{135300}{T [K]} + 2 \right) \exp \left(\frac{47800}{T [K]} \right) [m^6 / (mol^2 \cdot s)]$$

Radiative recombination to the ground state



is taken into account with a rate coefficient (K_{2+}) derived from data in [9]. This process represents the main radiative energy loss in the free-burning arc. The reverse process (photo-ionization) is not considered as a separate process. However, the continuum radiation can be partially trapped in the plasma. Therefore an escape factor A_{2+} as a function of the electron temperature [28] is introduced.

The model described so long has been further modified in two steps. First, an additional kind of species that groups the 4s excited states of neutral argon has been introduced into the transport of heavy particles. The model (referred to as "one level model") being modified in this way should be equivalent to the former one since the excited state had been implicitly considered in the overall reaction (see Eq. (1) and Eq. (2)). For that purpose the statistical weight of the effective excited level has been increased artificially by a factor of ten to ensure the particle flow to the continuum.

Secondly, higher excited levels have been considered. The four lowest excited levels 4s (1s₅, 1s₄, 1s₃, 1s₂ in Paschen notation) have been considered as individual species, the levels 2p₁₀-2p₅ have been grouped in an effective state, so have been 2p₄-2p₃ treated, too, 2p₂ and 2p₁ have been taken as individual, and an effective state (hl) has included further higher excited levels. The statistical weight of the hl group has been set to 200 to ensure the

particle flow to the continuum [7, 21]. This model will be referred to as “extended model” in what follows.

The ionization by electron impact is now taken into account using cross-section data from [29]. The excitation by electron impact is covered by the well adopted analytical forms by Drawin [17].

Inelastic atom-atom collisions are treated according to [13, 15] by means of cross-sections written as

$$\sigma_{ij}(\varepsilon) = \beta_{ij} \frac{\varepsilon - E_{ji}}{E_{ji}^{2.26}}, \quad (6)$$

where $E_{ji}=E(j)-E(i)$ is the energy gap between levels j and i ($j>i$), and β_{ji} is a level-dependent parameter. For excitation and ionization from the ground state, Eq. (6) is written as

$$\sigma_{ij}(\varepsilon) = \beta_{ij} (\varepsilon - E_{ji}). \quad (7)$$

For the radiative transitions, data recommended by Wiese et al. [30] is used. The transition probabilities A_{mn} (s^{-1}) between effective levels are calculated from the individual values as

$$A_{mn} = \frac{\sum_{j(m)} g_j \sum_{i(n)} A_{ji}}{\sum_{j(m)} g_j}, \quad (8)$$

where n and m denote the lower and the upper effective levels, and i and j correspond to the individual levels belonging to the lower and the upper effective level groups, respectively.

The radiative transport in the plasma is treated in terms of the Holstein escape factors for radiation [31] assuming that the plasma is optically thick for the resonance lines and optically thin for all other lines. This assumption is justified since the number density of the ground state is by orders of magnitude higher than the excited level densities. Then, the escape factors for all transitions but the resonance transitions are assumed to be equal to 1 (radiation trapping is neglected). For resonance transitions, the escape factors are estimated according to [31].

Under conditions typical for the present study, the ground state density of argon atoms is in the region $1 \cdot 10^{23}$ - $1 \cdot 10^{24} \text{ m}^{-3}$, the electron number density is about $1 \cdot 10^{22}$ - $1 \cdot 10^{23} \text{ m}^{-3}$, the gas temperature 10000 K-20000 K in the arc column with radius of about 1 cm. For the two resonance lines at 104.82 nm and 106.66 nm, the Lorentzian line broadening including a resonance, Stark, and Van der Waals broadening components, is about $1.5 \cdot 10^{-4} \text{ nm}$, the Doppler line broadening $1.5 \cdot 10^{-3} \text{ nm}$, and the resulting escape factor about $A=1 \cdot 10^{-3}$. Therefore, most of the resonance radiation is reabsorbed and only a small part of it can escape.

Surface reactions of neutralization ($\text{Ar}^* \rightarrow \text{Ar}$) and recombination ($\text{Ar}^+ \rightarrow \text{Ar}$) are considered on the boundaries fluid-solid in terms of the sticking coefficient approximation.

The procedure of resolving the excited states is aimed at obtaining level's densities which are related to emission lines under experimental observation. In the same time, the resolution of the excited states should not have influence on the main arc plasma parameters like electron and heavy particle temperatures, current density, electric potential. Therefore, keeping the arc plasma as it is in the simplest chemical model, a more detailed view into the distribution over excited levels would be enabled and correspondingly, a relation to data from emission spectroscopy could be established.

IV. RESULTS AND DISCUSSION

The simple model serves for useful purposes. It can be used as a fast track evaluation of the arc characteristics, sensitivity studies of the impact of model parameters, a variation of working conditions. In that way, the size of the cathode-arc attachment area has been determined using experimental data to compare the plasma temperatures in the hottest arc region for given arc current values.

Simulations have been performed according to the working conditions in Ch. II, i.e. arc current value of 200A and a gas flow rate of 12 slpm.

The radial distribution of the electron and heavy particle temperatures along a cut line between the cathode and the anode is shown as an example in Fig. 2. Experimental values obtained by means of emission spectroscopy of ArI and Ar II lines (at 696.5 nm and 488 nm, resp.) and assuming equilibrium composition [6] are also given. Without any restriction of the arc attachment area, the maximum temperature obtained in front of the cathode tip was slightly below 15000 K whereas temperatures of about 19000 K were expected according to experimental observations (Fig. 2a). A similar approach of adjusting the attachment area has been applied in [2]. Such a treatment is significant in arrangements with a conical electrode in order to obtain realistic temperatures in front of the cathode tip. Moving in direction to the anode (Fig. 2b), the differences between the temperatures values obtained with a restricted arc attachment and a free arc attachment reduce and remain for example below 2000 K being under circumstances still in the range of the experimental error bars as shown on the midline between the cathode and the anode.

Despite of the size of the arc attachment area, a common feature of the results obtained is the equal electron and heavy particle temperature in the arc body. A deviation from local thermodynamic equilibrium is observed as expected in the arc fringes where the electron temperature remains higher than the heavy particle temperature due to the low electron density and hence the low collision frequency there in.

In what follows, a comparison of the results of the various plasma chemistry models will be considered and discussed.

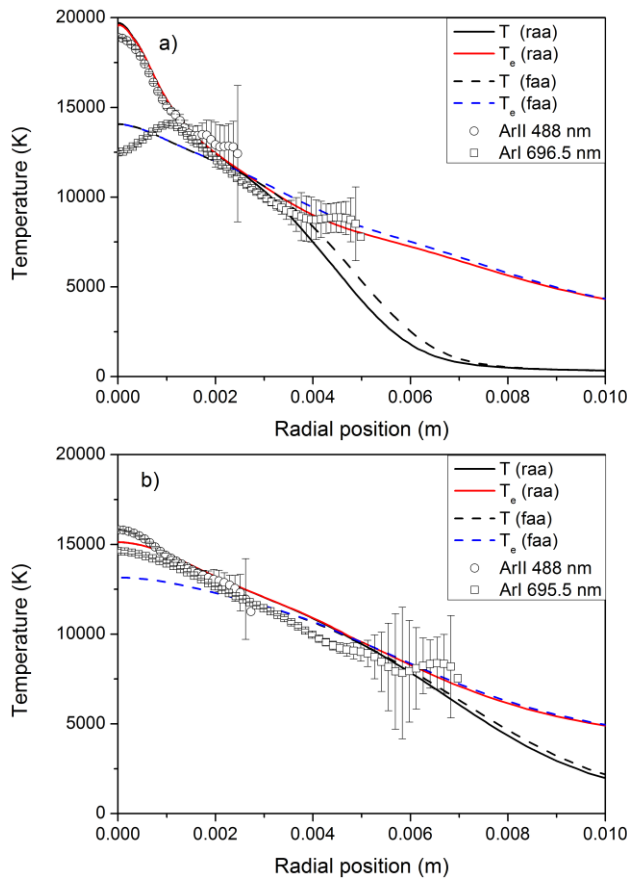


Figure 2. Electron and heavy particle temperatures along a cutline a) 1 mm and b) 4 mm away from the cathode. Symbols represent values from emission spectroscopy.

Fig. 3 presents the electron and heavy particle temperatures obtained with the three models. Despite the different reaction schemes and data applied the results obtained are close to each other. A significant deviation between the temperatures of heavy particles and electrons in the near-electrode regions (Fig. 3a). Extending the level-scheme leads to a slightly lower electron temperature in the arc fringes (Fig. 3b). A possible explanation of this effect concerns the additional losses of electron energy due to radiative recombination to the upper atomic levels which are not present in the simpler models.

Some deviations between the models appear in the radial profiles of the electron number density (Fig. 4). Note that here the arc fringes are plotted up to 0.02 m away from the axis in order to point out the differences. In the arc body the values deviate by not more than 5 % whereas in the far arc fringes it can be of one order of magnitude. Nevertheless it should be noted that this region (having electron number density values of $(10^{18}\text{--}10^{19})\text{ m}^{-3}$ compared to values of $(10^{22}\text{--}10^{23})\text{ m}^{-3}$ in the arc column does not contribute a lot to the whole arc picture. Differences in the electron number density found by the simple model and the one level model can be addressed to

the different data for ionization used. In the simple model the ionization has been described in terms of the prompt ionization approximation applying the forward rate coefficients given in Eq. (6) and Eq. (7). In the one level model, collisional cross-section data [17, 29] have been applied. Comparing the results of the one level model with the ones of the extended model, the small deviations occurring can probably be explained with the additional contribution of the upper excited levels.

In Fig. 4, the equilibrium and two-temperature (2-T) electron number density are also plotted. The equilibrium values are obtained with the heavy particle temperature T whereas the 2-T values make use of T and T_e from the extended non-equilibrium model. On the arc axis (Fig. 4a), the 2-T values agree well with the results of the non-equilibrium models being though a bit lower compared to the result of the extended model. Close to the cathode the 2-T values increase since surface reactions are not accounted for through the evaluation of the 2-T composition. The deviation from the equilibrium values is more significant. Perpendicular to the arc axis (Fig. 4b), the results of the non-equilibrium models deviate from both equilibrium and 2-T values for radial positions of 5 mm and beyond. Hence, the recombination rate coefficients which are probably proper in the arc column seem to be underestimated in the outer region.

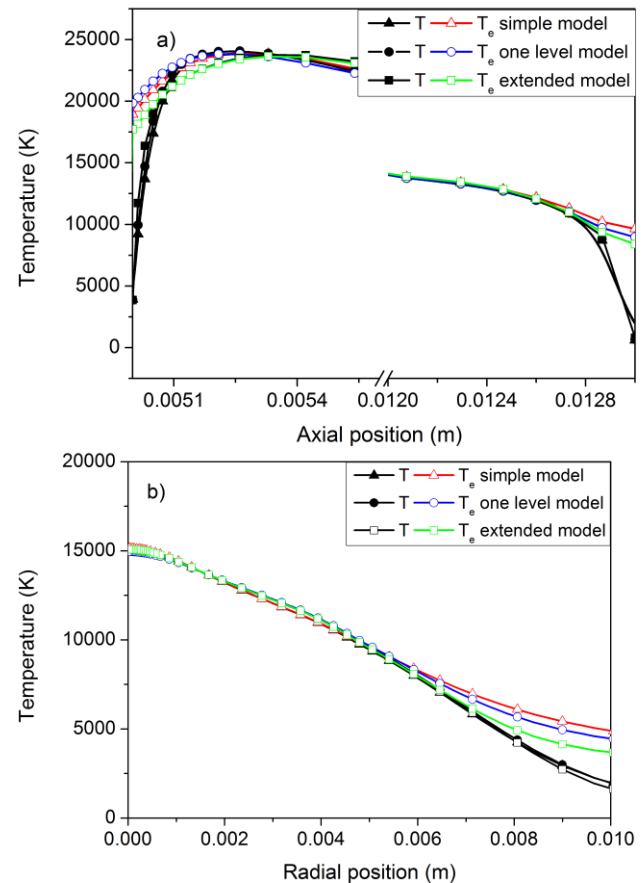


Figure 3. Electron and heavy particle temperatures along the arc axis a) and the midline (b).

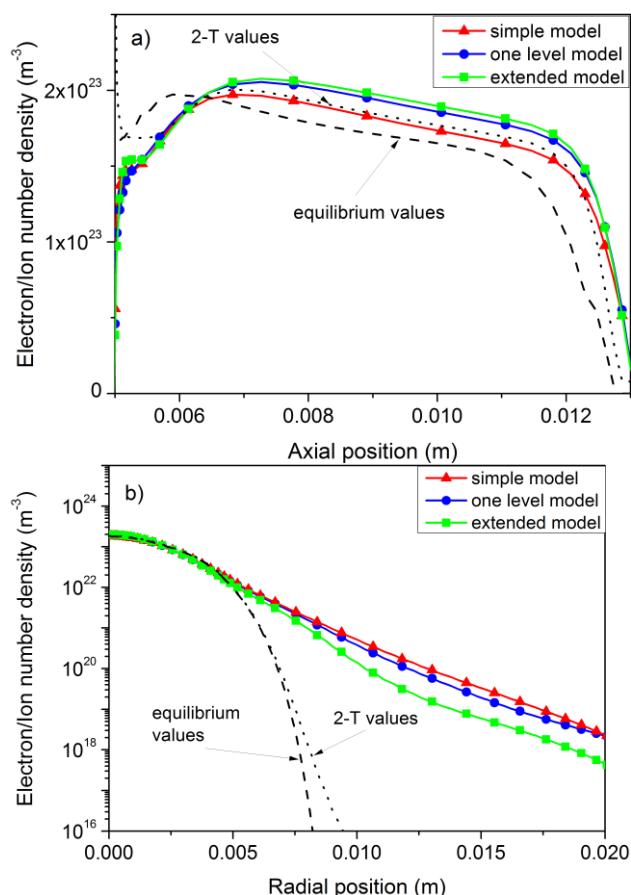


Figure 4. Electron density along a) the arc axis and b) a cut line in the midplane.

Let one consider the production terms of the three models along the midline between the cathode and the anode. Fig. 5 shows the corresponding reaction rates of the simple model (a), the one level model (b), and the extended model (c). In the simple model, the ionization of argon atoms appears from the ground state and implies excitation of the first excited state. The reaction rate achieves a maximum value of about 35 kmol/(m³.s) on the arc axis. The one level model considers an effective level composed by the four low lying excited states of the argon atom, i.e. three additional states are being involved. This model predicts that the reaction rate for ionization from the effective excited level (~45 kmol/(m³.s)) dominates over the reaction rate for ionization from the ground state (~1.3 kmol/(m³.s)). This result from one side justifies the approximation of prompt ionization, and from the other side shows that the simplified rate coefficients (Eq. (6)-(7)) are capable of predicting the ionization rate within 20% as compared to the more accurate collisional cross-section data applied in the one level model. Looking now at the results of the extended model as compared with the one level model, one can see that the deviations are small. The ionization rate from the excited states differs just in few percent which can be attributed to the contribution of the 4*p* and *h**l* levels provide that the

contribution of the 4*s* levels is equal. The dominating mechanism for loss of electrons in the arc plasma is the 3-body recombination. The reaction rate for radiative recombination in which the resulting atom is in the ground state is one order of magnitude

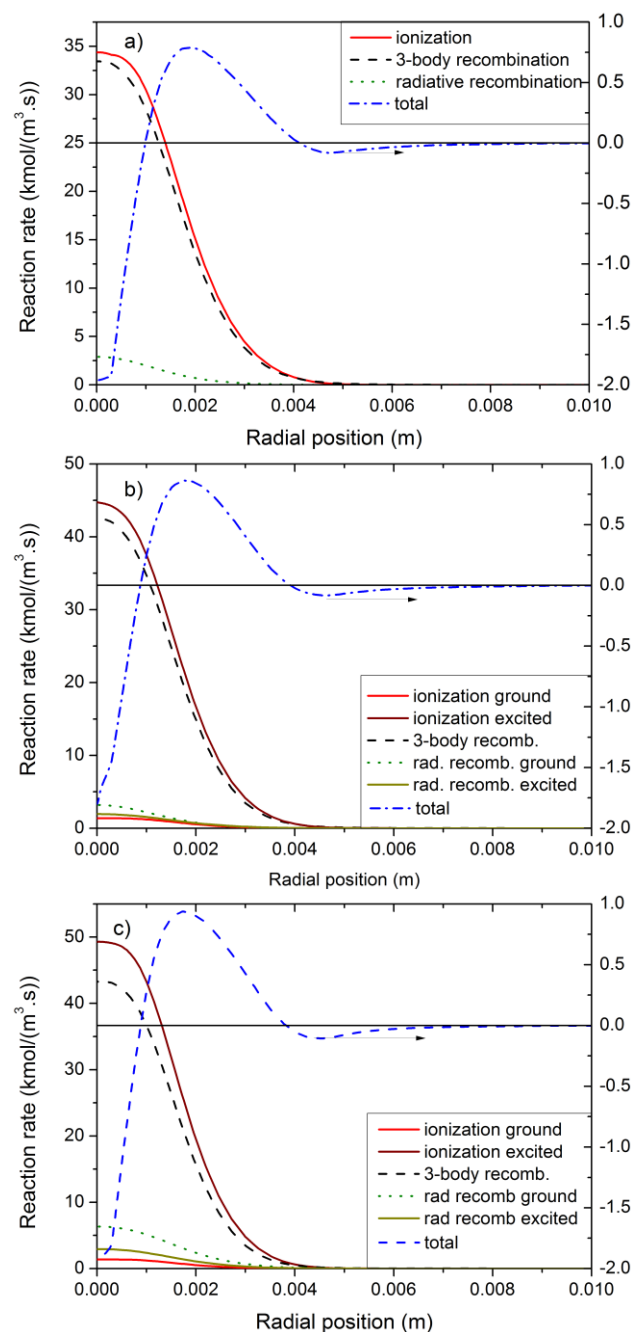


Figure 5. Reaction rates of production and loss of electrons along the midline obtained by means of: a) simple model, b) one level model, and c) extended model.

lower. The total reaction rate for radiative recombination of the ions to the excited states is about the half of that to the ground state. It should be noted that in the radiative recombination to the ground state a radiation trapping has

been accounted for whereas the continuum radiation resulting from radiative recombination to the excited states has been considered as optically thin [28], so that the inequality has been reduced.

Important result is the total production/loss rate of electrons plotted in Fig. 5 with the scale on the right side. The values of the total rate are very close to each other for the three models. This confirms that the bottleneck lies in the low excited states and therefore justifies the extended model. The absolute values being in the order of $1 \text{ kmol}/(\text{m}^3 \cdot \text{s})$ are low compared to the reaction rate for ionization itself but interesting is that the total reaction rate is changing the sign in radial direction. Close to the axis (radial position zero), the arc plasma has a net recombination, and then it shows a net ionization and turns again to net recombination before it comes to ionization-recombination equilibrium in the outer region.

The number density of the effective excited level in the one level model and the sum of number densities of levels $1s_5$ - $1s_2$ in the extended model is shown in Fig. 6 along the midline between the cathode and the anode. These densities are important for the ionization rate as discussed above. Both curves have the same course – they exhibit an off axis maximum at a radial position $\sim 1 \text{ mm}$ where the electron temperature is about 14000 K (Fig. 3) and so is being close to the levels' energy. The maximum values agree within 15%. The collisional cross-section data concerning the kinetics of the $4s$ levels is equal in so far the upper levels are kept beside. The only difference is in the statistical weights. It should be reminded that in the one level model the statistical weight of the effective level has been increased to ensure the particle flow to the continuum. In the extended model, the $4s$ levels are considered with their real statistical weights but the effective level hl has been prescribed an increased statistical weight. Another proper explanation shall be the contribution of the upper levels, e.g. emission from $4p$ and hl levels populating the $4s$ levels which is not considered in the frame of the one level model.

A weak second peak is observed in the outer region. The latter is apparently a result of 3-body recombination process. The secondary peak is present in the region in front of the anode and it is vanishing in direction to the cathode. Its position corresponds to the cold part of the arc fringes where the electron number density is still high ($\sim 10^{21}$ - 10^{22} m^{-3}) but the electron temperature is low enough (below 0.5 eV) so that the recombination rate coefficient is high. This process populates the $4s$ levels of the argon atom according to the reaction chemistry applied. Note that in the extended model the electron temperature is lower around a radial position 0.008 m (Fig. 3) so that the recombination rate coefficient is higher as compared to the simple model so that the secondary peak in the extended model is better pronounced.

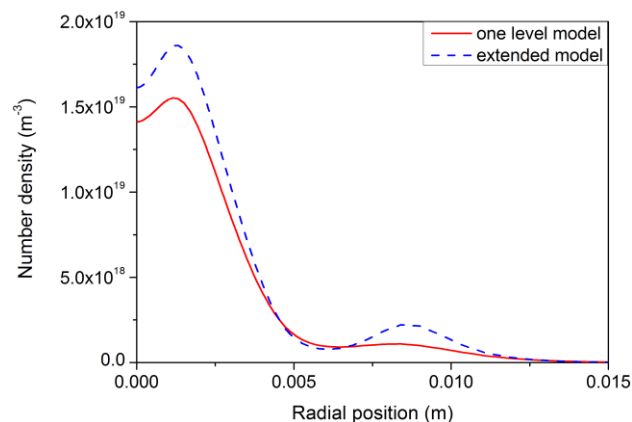


Figure 6. Population of the $4s$ states along the midline between the cathode and the anode.

V. SUMMARY

Reaction schemes with increasing number of excited states are considered in the non-equilibrium modelling of free-burning arc in argon. The role of the reaction chemistry on parameters like the temperatures of heavy particles and electrons, the ion production and loss rates, the electron number density is analyzed for an arc current of 200 A and an argon flow rate of 12 slpm . The self-consistent description unifies the arc plasma and the electrodes. The main results can be summarized as follows.

The simple model which is based on the assumption of prompt ionization delivers results which are very close to the results of the one level model which implies an effective excited level of argon atoms despite somewhat different reaction data have been applied.

The results obtained with all models show almost equal electron and heavy particle temperatures in the arc body and a significant deviation between the temperatures of heavy particles and electrons in the near-electrode regions and in the arc fringes. The most extended scheme demonstrates electron temperature in the arc fringes which is about 1400 K lower than the values obtained with the simple model. The deviation in the electron number density in the arc column does not exceed 5%. In the far arc fringes it can rise to an order of magnitude which is of minor importance concerning the total arc characteristics. The deviations occurring can probably be explained with the additional contribution of the upper excited levels.

The quantitative and qualitative agreement of the models enables a fast analysis of the main plasma parameters using a simple chemistry model. In addition, a detailed analysis of the excited level populations and emission spectra evaluation is possible applying the extended reaction chemistry at the expense of longer time of computation.

VI. REFERENCES

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